

INSIDE

2

From Alex's Desk

4

Meharchand named
American Physical
Society's Woman
Physicist of the Month

Insight on catalytic
behavior in hydrogen
catalyst weberites

5

New tool in the search
of a theory for Cu-based
superconductors

6

Journal's 80th
anniversary issue
features Lujan Neu-
tron Scattering Center
polymer study

7

Heads Up!

Celebrating service

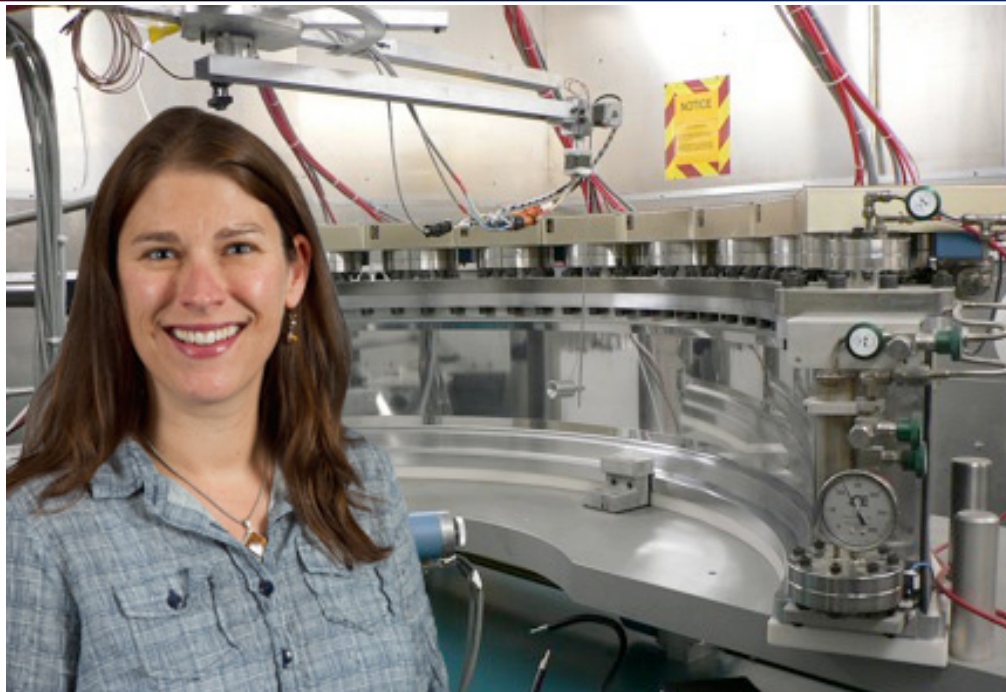


Photo by Sandra Valdez, IRM-CAS

Zoë Fisher studies enzymes in action in search of new ways to put them to use in far-ranging applications. She also assists visiting scientists to do the same at the Lujan Neutron Scattering Center's Protein Crystallography Station (pictured above).

“

From gene to final finished paper, we are heavily involved in all the steps. The behind-the-scenes work makes or breaks a project.

”

Zoë Fisher

Transforming enzymes before your very eyes

By Diana Del Mauro

ADEPS Communications

With a passion for science, Zoë Fisher seriously considered becoming a medical doctor, a fish farmer, or a winemaker in her South African homeland. But then she discovered biochemistry in college, and it was “magical” seeing in atomic detail how human bodies work, she said.

Today, as Fisher describes her research at Los Alamos's Lujan Neutron Scattering Center, she sounds a bit like a magician, waving a wand to line up proteins and enzymes and do as she commands. Produce algae for biofuels! Bind to the precise enzyme targeted for drug treatment! It's not magic, of course, but slow, painstaking work. A staff scientist in Bioenergy and Biome Sciences (B-11), Fisher investigates the mechanisms, structure, and function of enzymes—those life-sustaining protein molecules in blood.

With Harvard University scientists, for instance, Fisher is trying to deduce how water structure contributes to drug binding. In related work, she is studying enzyme action so drugs can be designed straight from the pharmaceutical

continued on page 3



From Alex's desk ...

Colleagues,

Let me first bring to your attention the *2012 LANSCE Activity Report*. As in past years, we report on major accomplishments of all LANSCE facilities—from science and technology advancements, to user operations and outreach activities, to major collaborations and capabilities advancements. The report, and accomplishments of course, could not be made possible without your continuing support, dedication, and contributions—and we thank you for that. I hope you enjoy reading it and hope the report will continue motivating you to contribute in the near future. Let me also take the opportunity to acknowledge the hard work of Elena Fernandez during the preparation of this report. The report can now be downloaded at lansce.lanl.gov/news/activityreport/LANSCE%20Activity%20Report%202012.pdf. Enjoy it!

As you may be aware, due to the government shutdown and the possible LANL operation shutdown that was presented last month, as a precaution we decided to cancel the 10th LANSCE Neutron School. The school is now scheduled to run January 6-15, 2014 and will be focused on scattering geosciences and materials in extreme environments. For additional information please visit lansce.lanl.gov/neutronschool/index.shtml.

We are continuing the CY13 run cycle and hosting users as planned—a lot of activities, and a lot of work to do. So please be attentive, cautious, and aware of your work environment. By the way, when you not too sure of the next steps, stop what you doing, think and never, never hesitate to ask and consult with your colleagues prior taking any additional action.

LANSCE Deputy Division Leader Alex Lacerda

“

The report, and accomplishments of course, could not be made possible without your continuing support, dedication, and contributions...

”

Alex

Fisher cont.

plant, rather than blindly screened for applications by synchrotrons, as now done by drug companies.

To perform these feats, she uses the Protein Crystallography Station (PCS). With neutrons produced at the Los Alamos Science Center (LANSCE), PCS reveals an atomic-level picture of enzymes, including water positions and hydrogen atom positions. Knowing the atom positions creates the possibility to alter these enzymes to perform better or even new tasks. Since coming on line in 2002, PCS, the first instrument of its kind to be built at a spallation neutron source, has inspired similar stations to be constructed throughout the world.

Fisher also manages the PCS team and user program, even growing crystal samples for visiting scientists in a busy support lab. “From gene to final finished paper, we are heavily involved in all the steps,” she said. “The behind-the-scenes work makes or breaks a project.”

All neutron crystal structures are deposited with the Protein Data Bank, a repository for biological macromolecular structures, and Fisher is proud that Los Alamos National Laboratory leads the world in contributions.

Leif Hanson, a University of Toledo assistant professor and one of the first PCS external users, has known Fisher since she was a graduate student. “She is a first-rate scientist. Quick and sharp are the adjectives I always think of (being) associated with her,” Hanson said. “Once you get ... up to speed to follow her, you realize that she is gearing down to try and communicate with you, her mind is moving that fast.”

Together they have been working to incorporate reliable low-temperature diffraction data measurements at PCS, a technique that will yield more detailed images. “This has been a surprisingly difficult process to implement and involves a convergence of large crystals, proper equipment, and available beam time,” Hanson said. “Zoë has been dogged in pursuing this functionality for PCS. I know it will happen because Zoë wants it to happen.”

When Fisher left South Africa to be a research scholar for a year at the University of Florida, she was unsure if her credentials would give her the chance to pursue her career in American institutions. She was amazed when her mentor, impressed by her performance, encouraged her to pursue a doctorate in molecular biology there.

While working with enzymes during her graduate studies Fisher became interested in neutrons. She attended the 2006 LANSCE School on Neutron Scattering. “I came to the neutron school and loved it,” Fisher said. “I loved the town. I loved the people. I loved the Lujan.” Fisher returned to Los Alamos as a postdoctoral researcher in 2007 and became a staff member in 2010.

Zoë Fisher's favorite experiment

What: This experiment isn't thrilling in terms of its scientific importance, but it was a deciding moment in my career path to neutrons.

When: I had been working towards optimizing crystals of carbonic anhydrase (CA) for neutron experiments but wasn't having a lot of success. A collaborator in France suggested that we perdeuterate CA as a way to boost signal-to-noise. She was successful in making perdeuterated CA for an x-ray experiment. I was very apprehensive that perdeuteration was going to change the CA active site compared to hydrogenous CA.

Where: This took place in 2005 when I was a graduate student in the lab of Professor Rob McKenna at the University of Florida.

How: I remember receiving the electronic data files and staying up late to refine the data enough to “see” the waters. The moment that I opened the maps, and was able to precisely superimpose the perdeuterated and hydrogenous CA crystal structures, was huge.

The aha moment: Right there, in the active site where the active site water network sits, the data were identical for the H₂O vs. D₂O structures. This was the proof of principle that a neutron structure was not only feasible but also relevant and artifact-free!

Meharchand named American Physical Society's Woman Physicist of the Month

For the benefit of young people considering scientific careers—particularly in physics—Rhiannon Meharchand (Neutron and Nuclear Science, LANSCE-NS) and co-editor Emma Ideal (Yale University) collected and self-published 35 essays by women American physicists, engineers, and chemists in *Blazing the Trail: Essays by Leading Women in Science*.

The American Physical Society's Committee on the Status of Women in Physics named Meharchand and Ideal the Woman Physicist of the Month for October/November for their work.

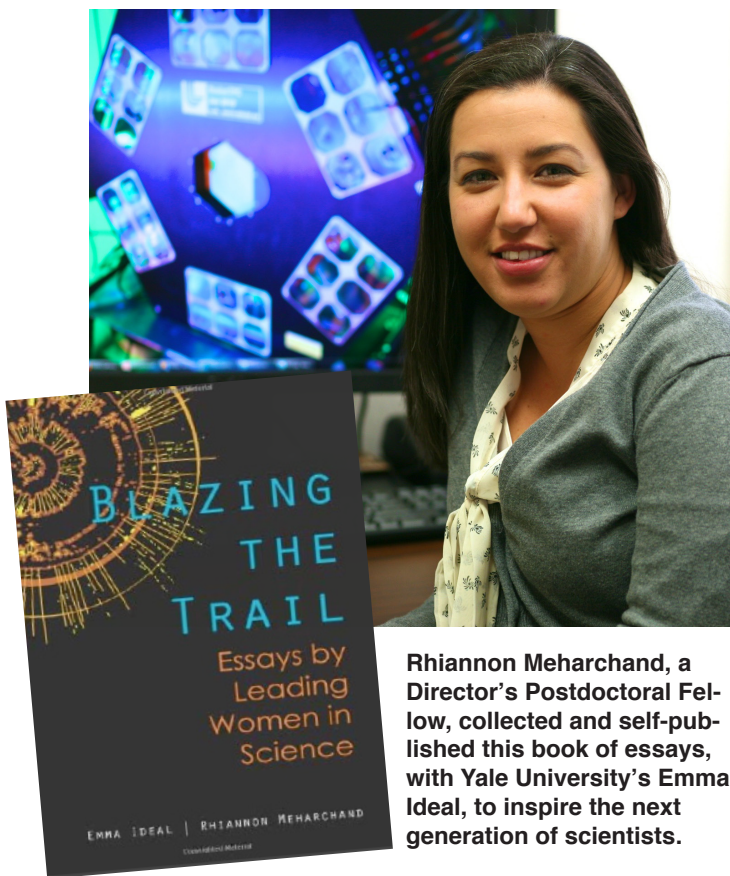
The collection of candid essays offers encouragement, career advice, and survival tips for the next generation. The combination of personal stories and advice sends a powerful message to all young women considering scientific careers: I did it, so can you. The preface reads: "The purpose of this book is threefold: to provide a diverse group of role models; to inform young people about scientific careers (physics in particular); and to encourage students to study science and pursue scientific careers."

Meharchand, a LANL Director's Postdoctoral Fellow, has previously been recognized for her mentoring accomplishments. As a Michigan State University (MSU) graduate student, she helped launch several student organizations, including a chapter of the Association for Women in Science (a national organization), and she received MSU's Sherwood K. Haynes Graduate Physics Award and an Outreach Award for co-founding the student organization Women and Minorities in the Physical Sciences. Meharchand also won the Association for Women in Science's Luise Meyer-Schutzmeister Memorial Award.

At Los Alamos, she plays a central part in a multi-institutional collaboration pursuing more precise measurements of plutonium-239, crucial for defense applications and for developing new fuels for fast nuclear reactors.

Christine Aidala, who was a Los Alamos Physics Division staff scientist at the time, wrote the book's first essay. Now at the University of Michigan, she studies the theory of the strong force, one of the three known fundamental forces in nature.

The American Physical Society's Committee on the Status of Women in Physics began the Woman Physicist of the Month program to highlight exceptional female physicists. The award recognizes female physicists who have positively impacted other individuals' lives and careers.



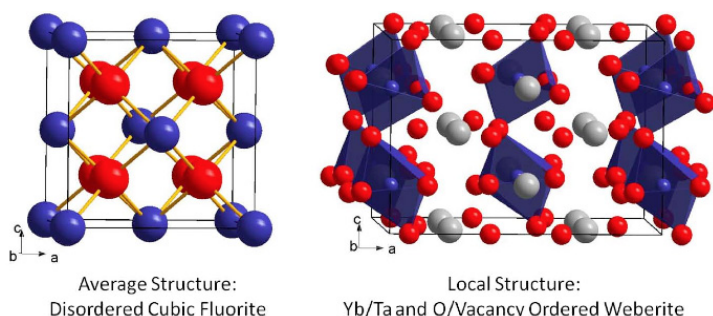
Rhiannon Meharchand, a Director's Postdoctoral Fellow, collected and self-published this book of essays, with Yale University's Emma Ideal, to inspire the next generation of scientists.

Insight on catalytic behavior in hydrogen catalyst weberites

Researchers used local structure analysis at the Lujan Neutron Scattering Center at Los Alamos National Laboratory to determine the difference in water splitting catalytic activity between weberites and defect fluorites. (weberite, $\text{Na}_2\text{MgAlF}_7$, is an orthorhombic mineral consisting of an aluminofluoride of sodium and magnesium.) La_3TaO_7 is an excellent catalyst for water splitting, while disordered Yb_3TaO_7 is not. By understanding why similar materials have different abilities to produce hydrogen from water, scientists could design new materials to enable a hydrogen-based economy.

The team determined that the local structure of Yb_3TaO_7 is weberite-like with short range ordering of cations and vacancies with domain sizes $\sim 30\text{\AA}$ long. This is much larger than the size of water molecules. Therefore, structure alone cannot explain differences in catalytic activity between this compound and those with long-range weberite structures. The structures of La_3TaO_7 and Yb_3TaO_7 are nearly the same on short length scales, but La_3TaO_7 has much greater long range order. In Yb_3TaO_7 there are many different Ta-O bond lengths, whereas the Ta-O bond lengths in La_3TaO_7 are more similar. The bond length difference may be related to the water splitting difference. Other structural differences, such as the degree of distortion of the Ta coordination environment, could also be responsible for the catalytic differences.

continued on next page



(Left): The average structure of Yb_3TaO_7 ; (right): the local structure.

Weberites cont.

Reference: “Local Structure of the Vacancy Disordered Fluorite Yb_3TaO_7 from Neutron Total Scattering,” *Journal of Materials Chemistry A* **1**, 10487 (2013). Researchers include G. King and A. Llobet (Lujan Center, LANSCE-LC), C. M. Thompson and J. E. Greedan (McMaster University, Canada).

This work benefited from the use of the high-resolution Neutron Powder Diffractometer at the Lujan Neutron Scattering Center at LANSCE, which the DOE Office of Basic Energy Sciences funds. The research supports the Lab’s Energy Security mission area and Materials for the Future and Science of Signatures science pillars.

Technical contact: Graham King

New discoveries on charge “stripes” in superconductors

Experiments performed on the Neutron Powder Diffractometer (NPDF) at Los Alamos have allowed scientists from Brookhaven National Laboratory to identify a series of clues that particular arrangements of electrical charges known as “stripes” may play a role in superconductivity—the ability of some materials to carry electric current with no energy loss. Stripe-like modulations of electronic states are presumed to be responsible for the superconductivity in Cu-based superconductors. Uncovering the detailed relationship between these stripe patterns and the appearance or disappearance of superconductivity has been extremely difficult, particularly because the stripes that may accompany superconductivity are very likely moving or fluctuating.

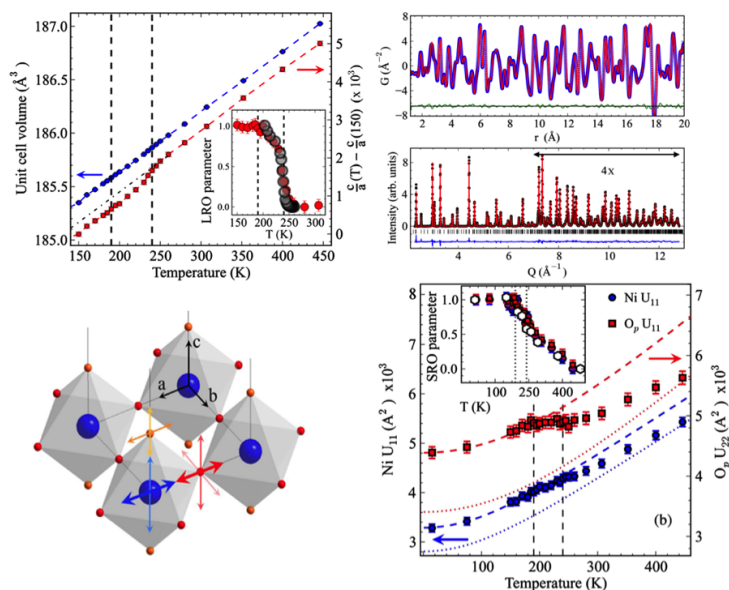
This work represents the first powder diffraction scattering evidence for fluctuating charge stripes above the temperature where static stripes develop. The polycrystalline sample— $\text{La}_{1.67}\text{Sr}_{0.33}\text{NiO}_4$ (LSNO)—is known to show robust charge-stripe order below 240 K. These results provide support for the idea that short-range-ordered, and presumably fluctuating, stripes could underlie electronic features, such as pseudogap and nematic and smectic phases seen in the related cuprates. *Physical Review Letters* published the work.

“One of the most critical aspects of this experiment is that we had lots of different data points, lots of temperatures—so you can catch small deviations,” said co-author Emil Bozin of Brookhaven. He also noted how improvements in detector technology made it possible to collect a lot of data within a fixed amount of time. “Ten years ago we would have needed a couple of weeks of beam time to do this experiment; we collected all our data in just a few days.”

The Lujan Neutron Scattering Center is a national user facility that attracts scientists from around the world. After a 2001 upgrade, NPDF became the first instrument of its kind designed specifically for pair distribution function analysis—a way of characterizing local atomic structure—and at the same time, it is among the best powder diffractometers in the United States for crystallographic analysis.

Reference: “Evidence for Short-Range-Ordered Charge Stripes Far above the Charge-Ordering Transition in $\text{La}_{1.67}\text{Sr}_{0.33}\text{NiO}_4$,” A.M.A. Abeykoon (Brookhaven National Laboratory) et al, *Physical Review Letters* **111**, 096404 (2013). This work was supported by the Office of Basic Energy Sciences, Division of Materials Sciences and Engineering, U.S. Department of Energy. This work benefited from the use of NPDF at the Los Alamos Neutron Science Center, funded by DOE Office of Basic Energy Sciences.

Technical contact: Katharine Page (NPDF Instrument Scientist)



Subtle changes in the c/a lattice parameter ratio in tetragonal LSNO at temperature T_{co} identify a structural signature sensitive to development of long-range static charge stripe order. On the other hand, excess magnitude of the ADPs above the canonical Debye characteristics correlates well with the pseudogap temperature evolution and is sensitive to short range ordered/fluctuating stripe correlations. Mean square displacements of Ni and O (extracted from Rietveld and PDF) along the Ni-O in-plane bond unveil a way to identify the existence of fluctuating stripes above T_{co} .

Journal's 80th anniversary issue features Lujan Neutron Scattering Center polymer study

To commemorate its 80th anniversary, the *Journal of Chemical Physics* selected 80 articles published in the journal over the past 80 years as highlights in chemical physics research. A landmark study of thin polymeric layers by Jarek Majewski (LANSCE-LC) and collaborators is featured in the 80th anniversary collection alongside articles by such renowned scientists as Paul Flory (Nobel laureate), Edward Teller, Nicholas Metropolis, and others. Thomson Reuters reports that the *Journal of Chemical Physics* is the most cited journal in atomic, molecular, and chemical physics.

Co-authored with four scientists from Kyoto University in Japan, the 2009 paper presented novel neutron measurements of polymer thin films. Widely used in everyday materials, polymer thin films consisting of single component and multicomponents are of great interest because their properties are quite different from bulk polymeric materials. Polymer thin films can be useful for coatings, adhesives, surface friction modifications, lubricants, and dielectric layers. Coatings can modify surfaces, for example, making them water repellant.

In this research, the scientists performed neutron scattering measurements to study the dewetting process of dPS/PVME (common polymers of polystyrene and poly-vinyl methyl ether) blend in the two-phase region. Dewetting describes the rupture of a thin liquid film on the substrate and the formation of droplets. The team used time-of-flight (or energy dispersive) neutron reflectometry to study the details of phase separation in the depth direction before dewetting. Neutron studies require high neutron fluxes. The Lujan Neutron Scattering Center, an international user facility, has one of the most intense sources of neutrons in the world. Majewski and Erik Watkins, his former student who is now at Institute Laue-Langevin in France, performed the measurements with the surface profile analysis reflectometer (SPEAR), which can study even the thinnest organic and inorganic layers in a variety of environments.

The researchers found that the phase separation of the two polymer components occurs near the air interface as well as near the silicon substrate during the incubation period before dewetting. The phase separation takes place asymmetrically at the two interfaces and progresses inhomogeneously along the film plane, indicating that a composition fluctuation mechanism induces dewetting. For the first time, the scientists analyzed the neutron off-specular data (neutrons scattered outside the main reflection region) to demonstrate that such measurements are very useful to investigate kinetics of structure formation in the film plane in the micrometer scale. The team learned that droplet formation in the micrometer scale happens in the late stage of dewetting. Their study showed that similar techniques could be used to address many other scientific problems.

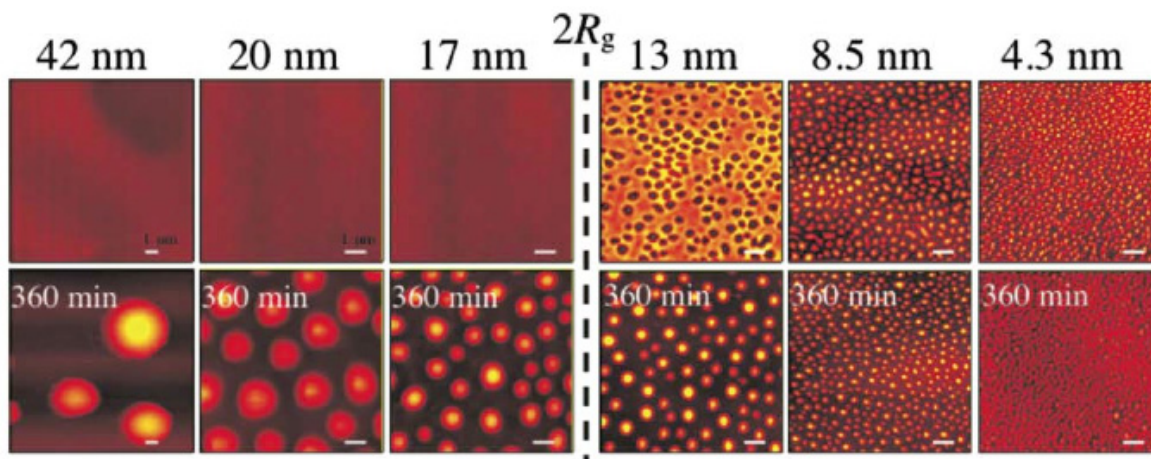
Reference: "Time-resolved Specular and Off-specular Neutron Reflectivity measurements on Deuterated Polystyrene and Poly(vinyl methyl ether) Blend Thin Films During Dewetting Process," *Journal of Chemical Physics* **131**, 104907 (2009). In addition to Majewski and Watkins, authors include Hiroki Ogawa, Toshiji Kanaya, Koji Nishida, and Go Matsuba (Kyoto University).

The DOE Office of Basic Energy Sciences sponsored the research at Los Alamos. The work benefited from the use of the Lujan Neutron Scattering Center at LANSCE funded by the DOE Office of Basic Energy Sciences. The research supports the Lab's Energy Security mission and Materials for the Future science pillar.

Technical contact: Jarek Majewski



Atomic force microscopy images of blend thin films before and after annealing at 115°C for 360 min for various initial film thicknesses above and below twice the radius of gyration (R_g) = 17 nm. Scale bars in images are 1 micron.



HeadsUP! How to help an ill or injured co-worker

Entering his office building early one Friday, Tom Archuleta (Plasma Physics, P-24) overheard a co-worker on his BlackBerry say he was having difficulty breathing. Archuleta noticed the man's hand was pressed against his chest. "It looked like he was having a heart attack," he said. The man, who prefers not to be identified, was sitting on the lobby couch, his face flushed.

Archuleta asked the man a series of questions to determine if he was having a heart attack. Did his arm hurt? Did he have pain or tightness in his chest? The man answered "no," but said he was struggling for air and his inhaler had not helped. Archuleta instructed another employee, Chris Lovejoy (International Threat Reduction, NEN-3), to call 911. Archuleta, Lovejoy, and NEN-3 Deputy Group Leader Rick Rasmussen stayed by the man's side until the arrival of paramedics, who administered medication and transported him to the Los Alamos Medical Center emergency room.

"I am feeling pretty good now," said the man, who had an allergic reaction that September day. "Looking back on the experience, it is very comforting to know that there are good people like Tom who look out for their fellow workers." He also expressed kind words of appreciation for Lovejoy and Rasmussen.

"It felt good to help him," Archuleta said. "It made my day!" Archuleta is trained in CPR, a requirement of his job, and has used his other life-saving skills outside of work, such as performing the Heimlich maneuver on a young adult choking at a restaurant. "The training that the Lab provides definitely prepared me to help out in those situations," he said.

Guidelines to follow

1.) Call 911 for assistance if the person's condition appears to be life threatening (such as a heart attack or severe allergic reaction), if moving the person could be detrimental (such as a neck injury or motor vehicle accident), or if the person requires the expertise and equipment of paramedics.

2.) If a person is unconscious have someone call 911 and start CPR only if you have proper training or find someone who does. Send another person to get an automated external defibrillator (AED). Determine if the person's breathing and pulse have ceased or seem irregular, then apply the AED immediately. Untreated sudden cardiac arrest causes death in minutes.

3.) Notify the worker's manager.

4.) Ensure all injuries and illnesses are reported to Occupational Medicine (OM) regardless of where the employee receives medical treatment. Call 667-0660, option 1. If a worker has an open wound in a Radiological Controlled area, remind the worker to report to OM to be examined.

5.) If the injury, illness, or exposure occurs either during off-hours or off-site, contact the on-call OM provider at 667-0660, option 1, for direction on where to report for evaluation and treatment.

For more information on when an employee needs medical care, see int.lanl.gov/employees/health-fitness/occupational-medicine/when-an-employee-needs-medical-care.shtml.

Celebrating service

Congratulations to the following LANSCE and AOT employees celebrating service anniversaries recently:

Jeffrey Hannaford, AOT-MDE.....	35 years
Richard Sheffield, LANSCE-DO	35 years
Tony Gomez, AOT-MDE	30 years
Alfred Maestas, AOT-MDE	30 years
John Faucett, AOT-IC	25 years
Robert Garnett, AOT-DO	25 years
John Harrison, AOT-RFE.....	15 years
Janet Lovato, AOT-RFE.....	15 years
Guenter Muhrer, LANSCE-LC	15 years
Trisha Gonzales, AOT-OPS.....	10 years
Kelly Knickerbocker, LANSCE-LC	5 years
Jeffrey Kolski, AOT-OPS	5 years
Elias Pulliam, AOT-HPE	5 years
Joan Siewenie, LANSCE-LC	5 years

thePulseAOT&LANSCE

Published by the Experimental Physical Sciences Directorate

To submit news items or for more information, contact Karen Kippen, ADEPS Communications, at 505-606-1822, or kippen@lanl.gov.

For past issues, see lansce.lanl.gov/news/pulse.shtml.



Los Alamos National Laboratory, an affirmative action/equal opportunity employer, is operated by Los Alamos National Security, LLC, for the National Nuclear Security Administration of the U.S. Department of Energy under contract DE-AC52-06NA25396. By acceptance of this article, the publisher recognizes that the U.S. Government retains a nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or to allow others to do so, for U.S. Government purposes. Los Alamos National Laboratory requests that the publisher identify this article as work performed under the auspices of the U.S. Department of Energy. Los Alamos National Laboratory strongly supports academic freedom and a researcher's right to publish; as an institution, however, the Laboratory does not endorse the viewpoint of a publication or guarantee its technical correctness.

LA-UR-13-28901

Approved for public release; distribution is unlimited.

Title: AOT & LANSCE The Pulse November 2013

Author(s): Kippen, Karen E.

Intended for: Newsletter
Web

Issued: 2013-11-19



Disclaimer:

Los Alamos National Laboratory, an affirmative action/equal opportunity employer, is operated by the Los Alamos National Security, LLC for the National Nuclear Security Administration of the U.S. Department of Energy under contract DE-AC52-06NA25396. By approving this article, the publisher recognizes that the U.S. Government retains nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or to allow others to do so, for U.S. Government purposes. Los Alamos National Laboratory requests that the publisher identify this article as work performed under the auspices of the U.S. Department of Energy. Los Alamos National Laboratory strongly supports academic freedom and a researcher's right to publish; as an institution, however, the Laboratory does not endorse the viewpoint of a publication or guarantee its technical correctness.